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Raman spectra and conformations of 2,2-dialkyl-1,3-dithio-5,6-benzocycloheptenes: coexistence of chair, boat and twist-boat forms

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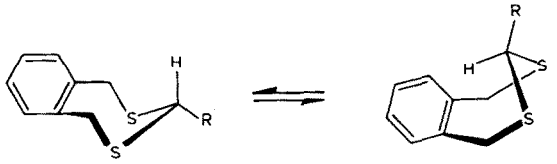
Abstract

Raman spectroscopy has been applied to the title compounds; dithiaketals of acetone, methylethylketone, pinacolone, cyclohexanone and fluorenone. A three-component chair⇌boat⇌twist-boat conformational equilibrium has been established for all compounds studied except the pinacolone derivative, which exhibits a two-component chair⇌boat equilibrium. Questions concerning the symmetry of the conformations based on depolarization data are discussed.

INTRODUCTION

Seven-membered dithiaacetals (**I**) are suitable models for investigation of chair (C) ⇌ boat (B) equilibria, and the analogous acetals (**II**) provide examples of chair⇌twist-boat (TB) equilibria.



(**I**) R=H,Me,Ph,*t*-Bu

Experimental data for dithiaketals of acetone (**III**) [1,2], cyclohexanone (**VI**) [2,3] and fluorenone (**VII**) [4] have made it possible to determine the

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